

Endothal
145-73-3 | DTXSID7024081

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.37

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 4.70e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Endothal</div> <div>Measured: 1.91</div> <div>Predicted: 1.37</div>	<div>Image not found</div> <div>Propanedioic acid, dimethyl-</div> <div>Measured: 0.39</div> <div>Predicted: 2.43e-01</div>	<div>Image not found</div> <div>Citric acid</div> <div>Measured: -1.64</div> <div>Predicted: -1.68</div>
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